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ScienceDirect
Linear Algebra and its Applications 430 (2009) 1566–1573
LINEAR ALGEBRA AND ITS APPLICATIONS
www.elsevier.com/locate/laa

Positive symmetric matrices with exactly one positive eigenvalue ☆

J.M. Peña

Departamento de Matemática Aplicada/IUMA, Universidad de Zaragoza, 50009 Zaragoza, Spain

Received 31 October 2007; accepted 8 April 2008
Available online 2 June 2008
Submitted by J. Moro

Abstract

Several properties of positive, symmetric matrices with exactly one positive eigenvalue are analyzed. They include their LDL^{T}-factorization as well as the growth factor of symmetric pivoting strategies applied to these matrices. An efficient test to check if a given positive, symmetric matrix has exactly one positive eigenvalue is presented. The relationship with other classes of matrices is analyzed.

AMS classification: 15A48; 15A23; 15A51; 65F05

Keywords: Symmetric matrices; Conditionally negative definite; Positivity; Growth factor

1. Introduction

The class of symmetric matrices with exactly one eigenvalue of one sign and the remaining eigenvalues of the other sign presents interesting properties. These matrices arise naturally in many areas: interpolation of scattered data, mathematical programming, numerical analysis and statistics (see [1,4]).

Following [1], the class of positive, symmetric matrices with exactly one positive eigenvalue will be denoted by $\mathscr{A}$. This paper will deal mainly with this class of matrices. Another related class of matrices is provided by the following definition. A real, symmetric $n \times n$ matrix A is

☆ Research partially supported the Spanish Research Grant MTM2006-03388, Gobierno de Aragón and Fondo Social Europeo.

E-mail address: jmpena@unizar.es

0024--379/$ - see front matter © 2008 Elsevier Inc. All rights reserved.
doi:10.1016/j.laa.2008.04.032

said to be *conditionally negative definite* if $x^{\mathrm{T}}Ax \leqslant 0$ for any $x = (x_1, \ldots, x_n)^{\mathrm{T}} \in \mathbf{R}^n$ such that $\sum_{i=1}^n x_i = 0$. By Corollary 4.1.5 of [1], if A is a positive, conditionally negative definite matrix, then $A \in \mathscr{A}$. By the equivalence of (1) and (10) of Theorem 4.4.6 of [1], a positive symmetric matrix $A \in \mathscr{A}$ if and only if the (unique) doubly stochastic matrix of the form $D^{\mathrm{T}}AD$ (where D is a diagonal matrix with positive diagonal entries) is conditionally negative definite. This stochastic matrix, which also belongs to $\mathscr{A}$, can be considered as the "normalization" of A.

In Section 3, we describe the LDL^{T}-factorization of nonsingular matrices in the class $\mathscr{A}$. In contrast, Example 3.2 shows that a symmetric negative nonsingular matrix with exactly one positive eigenvalue does not possess, in general, an LDL^{T}-factorization. Section 4 includes necessary and sufficient conditions for matrices in the class $\mathscr{A}$. In particular, we focus on the normalized version mentioned above, which corresponds to stochastic matrices. In this case, we prove that $\mathscr{A}$ contains the class of C-matrices introduced in [8]. This last class of matrices has been used to obtain exclusion intervals for the real eigenvalues of a real matrix.

The growth factor of a numerical algorithm is usually defined as the quotient between the maximal absolute value of all the elements that occur during the performance of the algorithm and the maximal absolute value of all the initial data. A small growth factor avoids overflows and is an indicator of stability and robustness. In particular, it is well known that the stability of an elimination procedure to transform a nonsingular matrix into an upper triangular matrix depends on the corresponding growth factor (see [3]). In Section 5, we analyze the growth factors of symmetric pivoting strategies applied to matrices in the class $\mathscr{A}$. We find pivoting strategies with minimal growth factor. We also propose an efficient test to check if a given positive, symmetric nonsingular matrix belongs to $\mathscr{A}$. This test presents a small growth factor. Other recent tests for other classes of matrices also present a small growth factor (see [2,6,7]).

2. Basic notations

In this paper, we say that a matrix is *positive* (respectively, *nonnegative*) if all its entries strictly positive (respectively, nonnegative). A nonnegative matrix $A = (a_{ij})_{1 \leqslant i,j \leqslant n}$ is called *stochastic* if, for all $i = 1, \ldots, n$, $\sum_{j=1}^n a_{ij} = 1$. If A and A^{T} are stochastic, then we say that A is *doubly stochastic*. We say that a symmetric matrix is negative definite if $x^{\mathrm{T}}Ax < 0$ for any $x \neq 0$. It is well known that a $k \times k$ principal submatrix of a negative definite matrix has determinant with sign $(-1)^k$.

Given $k \in \{1, 2, \ldots, n\}$, let α, β be two increasing sequences of k positive integers less than or equal to n. Then we denote by $A[\alpha|\beta]$ the $k \times k$ submatrix of A containing rows numbered by α and columns numbered by β. For principal submatrices, we use the notation $A[\alpha] := A[\alpha|\alpha]$.

Gaussian elimination with a given pivoting strategy, for nonsingular matrices $A = (a_{ij})_{1 \leqslant i,j \leqslant n}$, consists of a succession of at most $n-1$ major steps resulting in a sequence of matrices as follows:

$$A = A^{(1)} \longrightarrow \widetilde{A}^{(1)} \longrightarrow A^{(2)} \longrightarrow \widetilde{A}^{(2)} \longrightarrow \cdots \longrightarrow A^{(n)} = \widetilde{A}^{(n)} = DU, \tag{2.1}$$

where $A^{(t)} = (a_{ij}^{(t)})_{1 \leqslant i,j \leqslant n}$ has zeros below its main diagonal in the first $t-1$ columns and DU is upper triangular with the pivots on its main diagonal. The matrix $\widetilde{A}^{(t)} = (\tilde{a}_{ij}^{(t)})_{1 \leqslant i,j \leqslant n}$ is obtained from the matrix $A^{(t)}$ by reordering the rows and/or columns $t, t+1, \ldots, n$ of $A^{(t)}$ according to the given pivoting strategy and satisfying $\tilde{a}_{tt}^{(t)} \neq 0$. To obtain $A^{(t+1)}$ from $\widetilde{A}^{(t)}$ we produce zeros in column t below the *pivot element* $\tilde{a}_{tt}^{(t)}$ by subtracting multiples of row t from the rows beneath it. Rows $1, 2, \ldots, t$ are not altered, according to the formula

$$a_{ij}^{(t+1)} = \begin{cases} \tilde{a}_{ij}^{(t)} & \text{if } i \leqslant t, \\ \tilde{a}_{ij}^{(t)} - (\tilde{a}_{it}^{(t)}/\tilde{a}_{tt}^{(t)})\tilde{a}_{tj}^{(t)} & \text{if } i \geqslant t+1 \text{ and } j \geqslant t+1, \\ 0 & \text{otherwise.} \end{cases} \tag{2.2}$$

We say that we carry out a *symmetric pivoting strategy* when we perform the same row and column exchanges. In this case, $PAP^{\mathrm{T}} = LDU$, where L (respectively, U) is a lower (respectively, upper) triangular matrix with unit diagonal and P is the permutation matrix associated to the pivoting strategy. For brevity, we shall call unit triangular matrix to a triangular matrix with unit diagonal.

3. LDL^{T}-factorization

In this section, we characterize matrices in $\mathscr{A}$ in terms of their LDU-factorization (LDL^{T}-factorization by symmetry). The result cannot be extended analogously to other classes of symmetric matrices with exactly one eigenvalue of one sign and the remaining eigenvalues of the other sign, as Example 3.2 shows.

Theorem 3.1. *Let $A = (a_{ij})_{1\leqslant i,j\leqslant n}$ be a positive nonsingular matrix. Then $A \in \mathscr{A}$ if and only if $A = LDL^{\mathrm{T}}$, where L is a unit lower triangular matrix and D is a nonsingular diagonal matrix with the first diagonal entry positive and all remaining diagonal entries negative.*

Proof. Let us assume that A has an LDL^{T}-decomposition with the properties of the statement. Then it is symmetric and has exactly one positive eigenvalue by Sylvester's law of inertia because it is congruent with D. Therefore, $A \in \mathscr{A}$.

Let us now assume that the positive nonsingular matrix A belongs to $\mathscr{A}$. Since $a_{11} \neq 0$, we can perform a first step of Gauss elimination and obtain the matrix $A^{(2)}$ of (2.1). Let L_1 be the unit lower triangular matrix associated to this step of Gauss elimination, that is, $L_1 A = A^{(2)}$. Then the matrix $B := L_1 A L_1^{\mathrm{T}}$ has the vector $(a_{11}, 0, \ldots, 0)$ as the first row (and column) and so it has the positive eigenvalue a_{11}. Observe also that we can write $B = A^{(2)} L_1^{\mathrm{T}}$ and so the matrix L_1^{T} transforms $A^{(2)}$ by adding to each column a multiple of the first one. Hence $B[2, \ldots, n] = A^{(2)}[2, \ldots, n]$. Since B is congruent with A, it has by Sylvester's law of inertia $n-1$ negative eigenvalues, which are the eigenvalues of $B[2, \ldots, n] = A^{(2)}[2, \ldots, n]$. Therefore $A^{(2)}[2, \ldots, n]$ is negative definite and it is well known (cf. p. 342 of [9]) that we can continue its Gauss elimination (and so, that of A) without row or column exchanges. In conclusion, we can perform the LDU-factorization of A, and since it is symmetric, we can write $A = LDL^{\mathrm{T}}$, where L is a unit lower triangular matrix and D is a nonsingular diagonal matrix. Since D is congruent with A, again by Sylvester's law of inertia D has one positive eigenvalue and $n-1$ negative eigenvalues. $\square$

The following example shows that a similar result to Theorem 3.1, but changing positive matrix by negative matrix, does not hold because a negative nonsingular matrix with exactly one positive eigenvalue does not necessarily have an LDL^{T}-factorization.

Example 3.2. Let A be the matrix

$$A = \begin{pmatrix} -1 & -1 & -1 \\ -1 & -1 & -2 \\ -1 & -2 & -3 \end{pmatrix}.$$

The matrix is symmetric, negative and nonsingular with $\det A = 1$. The positivity of the determinant (whose value is the product of the eigenvalues) and the negativity of the trace (whose value coincides with the sum of the eigenvalues) imply that A has exactly one positive eigenvalue. But A does not possess an LDL^{T}-factorization because its leading principal submatrix $A[1,2]$ is singular.

4. Necessary and sufficient conditions for stochastic matrices

As the following result shows, an off-diagonal dominance is a necessary condition for matrices in the class $\mathscr{A}$.

Proposition 4.1. *If $A = (a_{ij})_{1\leqslant i,j\leqslant n} \in \mathscr{A}$, then*

$$a_{ij} \geqslant \min\{a_{ii}, a_{jj}\}, \quad i \neq j. \tag{4.1}$$

Proof. Let us assume that there exist indices $i \neq j$ such that $a_{ij} < \min\{a_{ii}, a_{jj}\}$. Then $\det A[i, j] = a_{ii}a_{jj} - a_{ij}^2 > 0$. This contradicts the fact that, by the equivalence of (1) and (10) of Theorem 4.4.6 of [1], all 2×2 principal submatrices of a matrix in $\mathscr{A}$ have nonpositive determinant. $\square$

The following example shows that the previous condition (4.1) is not sufficient for a matrix to belong to $\mathscr{A}$.

Example 4.2. Let A be the matrix

$$A = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & \varepsilon \\ 1 & \varepsilon & \varepsilon \end{pmatrix}$$

with $0 < \varepsilon < 1/2$. The matrix is symmetric, positive and (4.1) holds. However, $A \notin \mathscr{A}$ because $\det A < 0$.

We have recalled in Section 1 that, given a matrix $A \in \mathscr{A}$, we can obtain a stochastic matrix, which also belongs to $\mathscr{A}$ and which is conditionally negative definite. From now on, we shall focus on stochastic matrices in $\mathscr{A}$ or, more generally, positive matrices in $\mathscr{A}$ which are multiple of stochastic matrices. Let us start with a strong off-diagonal dominance property which provides a sufficient condition to assure that a symmetric positive matrix which is a multiple of a stochastic matrix belongs to $\mathscr{A}$.

Proposition 4.3. *If $A = (a_{ij})_{1\leqslant i,j\leqslant n}$ is a symmetric positive matrix multiple of a stochastic matrix and satisfying for all $i = 1, \dots, n$*

$$a_{ij} > \frac{r}{n} \quad \forall j \neq i, \tag{4.2}$$

where r is the row sum of A (that is, $r := \sum_{k=1}^{n} a_{ik}$ for all i), then $A \in \mathscr{A}$.

Proof. If $e := (1, \dots, 1)^{\mathrm{T}}$, observe that $Ae = re$ and so r is a positive eigenvalue of A. Since A is irreducible, by Theorem 4.3 of Chapter 1 of [5] the eigenvalue r has algebraic multiplicity 1. Then, by Proposition 2.6 of [8], the remaining eigenvalues of A do not belong to the interval

$$\left(\max_{i=1,\dots,n} \{r - ns_i^+\}, \min_{i=1,\dots,n} \{r - ns_i^-\} \right), \tag{4.3}$$

where $s_i^+ := \max\{0, \min\{a_{ij} | j \neq i\}\}$ and $s_i^- := \min\{0, \max\{a_{ij} | j \neq i\}\}$. Since A is positive and (4.2) holds, we deduce that, in this case, $s_i^- = 0$ and $ns_i^+ > r$. Therefore, the interval of (4.3) contains the interval $[0, r)$ and we conclude that r is the unique positive eigenvalue of A. $\square$

Definition 2.1 of [8] introduces the concept of C-matrix: a square real matrix $A = (a_{ik})_{1\leqslant i,k\leqslant n}$ with positive row sums is a *C-matrix* if all its off-diagonal elements are bounded bellow by the corresponding row means, i.e., for all $i = 1, \ldots, n$

$$\sum_{k=1}^{n} a_{ik} > 0 \quad \text{and} \quad \frac{1}{n}\left(\sum_{k=1}^{n} a_{ik}\right) < a_{ij} \quad \forall j \neq i. \tag{4.4}$$

Observe that, if A is a positive matrix multiple of a stochastic matrix and $r := \sum_{j=1}^{n} a_{ij}$ for all i, then conditions (4.4) are equivalent to (4.2) (and the trivial condition $r > 0$). In conclusion, the following corollary holds:

Corollary 4.4. *If $A = (a_{ij})_{1\leqslant i,j\leqslant n}$ is a symmetric positive stochastic C-matrix, then $A \in \mathscr{A}$.*

The following example shows that the condition (4.2) is not necessary for a matrix to belong to $\mathscr{A}$.

Example 4.5. Let A be the matrix

$$A = \begin{pmatrix} 1/5 & 1/5 & 3/10 & 3/10 \\ 1/5 & 1/10 & 3/10 & 2/5 \\ 3/10 & 3/10 & 3/20 & 1/4 \\ 3/10 & 2/5 & 1/4 & 1/20 \end{pmatrix}.$$

The matrix A is symmetric, positive and stochastic, but (4.2) does not hold for $i = 1$, $j = 2$: $1/5 \leqslant r/4 = 1/4$. However, the matrix belongs to $\mathscr{A}$ by Theorem 3.1. In fact, it can be checked that $A = LDL^{\mathrm{T}}$ with

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 3/2 & -1 & 2/3 & 1 \end{pmatrix}, \quad D = \begin{pmatrix} 1/5 & 0 & 0 & 0 \\ 0 & -1/10 & 0 & 0 \\ 0 & 0 & -3/10 & 0 \\ 0 & 0 & 0 & -1/6 \end{pmatrix}.$$

Example 4.2 has shown that condition (4.1) is not sufficient for a matrix to belong to $\mathscr{A}$. The next example shows that this still holds even for stochastic matrices.

Example 4.6. Let A be the matrix

$$A = \begin{pmatrix} 1/5 & 1/5 & 3/10 & 3/10 \\ 1/5 & 1/10 & 3/10 & 2/5 \\ 3/10 & 3/10 & 1/4 & 3/20 \\ 3/10 & 2/5 & 3/20 & 3/20 \end{pmatrix}.$$

The matrix is symmetric, positive, stochastic and (4.1) holds. However, $A \notin \mathscr{A}$ because $\det A > 0$.

Let us finish this section by observing that a symmetric positive matrix $A \in \mathscr{A}$ has positive trace, which implies that the positive eigenvalue λ_1 and the negative eigenvalues λ_j $(j > 1)$ satisfy

$$\lambda_1 > \sum_{j=2}^{n} |\lambda_j|. \tag{4.5}$$

If A is, in addition stochastic, we derive $1 > \sum_{j=2}^{n} |\lambda_j|$.

5. Minimal growth factor and a stable test

Using the notation of formula (2.1) in Section 2, let us recall that if A is an $n \times n$ nonsingular matrix such that we can perform the Gaussian elimination of A with a given pivoting strategy, then the growth factor of A is the number

$$\rho_n(A) := \frac{\max_{i,j,k}\{|a_{ij}^{(k)}|\}}{\max_{i,j}\{|a_{ij}|\}}. \tag{5.1}$$

Theorem 5.1. *Let $A = (a_{ij})_{1\leqslant i,j\leqslant n}$ be a nonsingular matrix such that $A \in \mathscr{A}$. Let us suppose that we apply Gaussian elimination with a symmetric pivoting strategy and that a_{jj} is the first pivot. Then the growth factor $\rho_n(A)$ is given by*

$$\rho_n(A) = \max\left\{\max_{i\neq j}\left\{\frac{a_{ij}^2}{a_{jj}\max_{h\neq k}\{a_{hk}\}} - \frac{a_{ii}}{\max_{h\neq k}\{a_{hk}\}}\right\}, 1\right\}. \tag{5.2}$$

Proof. Let P be the permutation matrix associated to the symmetric pivoting strategy and let $B := P^{\mathrm{T}}AP$. Then we can perform Gaussian elimination of B without row and column exchanges. Following the notation of formula (2.1), we know that the matrices $B^{(k)}$ ($k \leqslant n$) obtained with Gaussian elimination of B without row and column exchanges coincide with the corresponding matrices $\widetilde{A}^{(k)}$ up to simultaneous permutations of rows and columns. Therefore, the growth factors coincide: $\rho_n(A) = \rho_n(B)$. Since B is congruent to A, B is also a nonsingular matrix which belongs to $\mathscr{A}$.

Let us now prove that

$$\max_{2\leqslant i,j,k\leqslant n}\{|b_{ij}^{(k)}|\} = \max_{2\leqslant i\leqslant n}\{|b_{ii}^{(2)}|\}\left(= \max_{2\leqslant i\leqslant n}\{|a_{ii}^{(2)}|\}\right). \tag{5.3}$$

Since B is a nonsingular matrix which belongs to $\mathscr{A}$, by Theorem 3.1 $B = LDL^{\mathrm{T}}$, where L is a unit lower triangular matrix and D is a nonsingular diagonal matrix with the first diagonal entry positive and all remaining diagonal entries negative. Observe that $B^{(2)}[2,\ldots,n] = L[2,\ldots,n]D[2,\ldots,n]L^{\mathrm{T}}[2,\ldots,n]$. Hence $B^{(2)}[2,\ldots,n]$ is congruent to a diagonal negative definite matrix and so it is also negative definite. Then formula (5.3) follows from the known property for negative definite matrices which claims that the diagonal entry with maximal absolute value has also an absolute value greater than or equal to that of the remaining entries of all matrices appearing in the Gaussian elimination of the matrix, but we provide a sketch of the proof of this fact for the sake of completeness. The positivity of all 2×2 principal minors of the negative definite matrix $B^{(2)}[2,\ldots,n]$ implies that its entry with maximal absolute value is a diagonal entry. This also happens to the matrix $B^{(3)}[3,\ldots,n]$, which is also definite negative. Taking into account that the diagonal entries of $B^{(2)}[2,\ldots,n]$ are negative, the symmetry of the matrix and formula (2.2), we can deduce that all diagonal entries of $B^{(3)}[3,\ldots,n]$ have less absolute value than the corresponding entries of $B^{(2)}[2,\ldots,n]$. Continuing the same argument with the remaining matrices $B^{(4)}[4,\ldots,n],\ldots,B^{(n-1)}[n-1,n]$, $B^{(n)}[n]$, the claim follows.

Let us now observe that the numbers of the set $\{b_{22}^{(2)}, \ldots, b_{nn}^{(2)}\} = \{a_{22}^{(2)}, \ldots, a_{nn}^{(2)}\}$ are, by (2.2), of the form

$$a_{ii} - \frac{a_{ij}^2}{a_{jj}}, \quad i = 2, \ldots, n. \tag{5.4}$$

From Proposition 4.1, we deduce that the denominator of formula (5.1) is given by the number $\max_{h \neq k}\{a_{hk}\}$. If $\max_{i,j,k}\{|a_{ij}^{(k)}|\}$ is achieved for $k > 1$, then the numerator of the formula (2.1) for the growth factor $\rho_n(A)$ is the maximum of the diagonal entries of $A^{(2)}[2, \ldots, n]$ (which are formed by the elements of (5.4)) and, if $\max_{i,j,k}\{|a_{ij}^{(k)}|\}$ is achieved for $k = 1$, then $\rho_n(A) = 1$, and the result follows. $\square$

Remark 5.2. In general, calculating the growth factor $\rho_n(A)$ of applying Gaussian elimination with a given pivoting strategy to an $n \times n$ matrix A requires $\mathscr{O}(n^3)$ elementary operations, due to the comparison of the absolute values of the entries of $A, A^{(2)}[2, \ldots, n], \ldots, A^{(n-1)}[n-1, n], A^{(n)}[n]$. By Theorem 5.1, the growth factor of *all* symmetric pivoting strategies of $A \in \mathscr{A}$ can be calculated with $\mathscr{O}(n^2)$ elementary operations corresponding to the n possibilities of j in Theorem 5.1. In fact, it requires $n(n-1)$ subtractions, n^2 divisions, $n(n+1)/2$ products and $(3(n^2-n)+2)/2$ comparisons. Moreover, we can identify the pivoting strategy with minimal growth factor with a low computational cost. If one only wants to choose a pivoting strategy with small growth factor, observe that, by Proposition 4.1

$$\frac{a_{ij}^2}{a_{jj}\max_{h \neq k}\{a_{hk}\}} \geqslant \frac{a_{ij}^2}{a_{jj}\max_{h \neq k}\{a_{hk}\}} - \frac{a_{ii}}{\max_{h \neq k}\{a_{hk}\}} \geqslant \frac{a_{ij}^2}{a_{jj}\max_{h \neq k}\{a_{hk}\}} - 1$$

and so, by (5.2), the growth factor $\rho_n(A)$ belongs to the interval

$$\left[\max_{i \neq j}\left\{\frac{a_{ij}^2}{a_{jj}\max_{h \neq k}\{a_{hk}\}}\right\} - 1, \max\left\{\max_{i \neq j}\left\{\frac{a_{ij}^2}{a_{jj}\max_{h \neq k}\{a_{hk}\}}\right\}, 1\right\}\right]. \tag{5.5}$$

Then, in order to obtain a symmetric pivoting strategy with small growth factor, we can slightly reduce the previous computational cost by looking for the index $j \in \{1, \ldots, n\}$ that minimizes

$$\max_{i \neq j}\left\{\frac{a_{ij}^2}{a_{jj}}\right\}. \tag{5.6}$$

The corresponding computational cost is now $n(n-1)$ divisions, $n(n-1)/2$ products and n^2 comparisons. Taking into account that the interval of (5.5) has length less than or equal to 1, any symmetric pivoting strategy choosing as first pivot index j minimizing (5.6) has a growth factor which exceeds at most 1 over the minimal growth factor among all symmetric pivoting strategies.

The proof of Theorem 5.1 and the previous remark suggest an efficient test to check if a given positive, symmetric nonsingular matrix belongs to $\mathscr{A}$. The test has the following steps:

- Choose as first pivot a_{jj} with $j \in \{1, \ldots, n\}$ minimizing (5.6) and obtain $\widetilde{A}^{(1)}$ (by exchanging rows and columns 1 and j) and $A^{(2)}$ with Gaussian elimination (see (2.1)). If $A^{(2)}[2, \ldots, n]$ has a nonnegative diagonal entry, then it cannot be negative definite and $A \notin \mathscr{A}$. Otherwise, we continue with the following step.
- Perform Gauss elimination to $A^{(2)}[2, \ldots, n]$ without row or column exchanges. If any diagonal entry of any of the matrices $A^{(3)}[3, \ldots, n], \ldots, A^{(n-1)}[n-1, n], A^{(n)}[n]$ is nonnegative, then $A \notin \mathscr{A}$. Otherwise, $A \in \mathscr{A}$.

In the worst case, the computational cost of the previous test increases the cost of Gaussian elimination in at most $n(n-1)$ divisions, $n(n-1)/2$ products and n^2 comparisons.

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